CONTENTS

Extension of AM1 to the halogens
M.J.S. Dewar and E.G. Zoebisch (Austin, TX, U.S.A.) 1

Calculations on the electron affinities of the phosphorus atom and its hydrides (PH_n, n=0–4)
M.T. Nguyen (Groningen, The Netherlands) 23

Valence bond analysis of molecular orbital wavefunctions: the ionicity of the $B^1\Sigma_u^+$ state of H_2
P. Karafiloglou (Thessaloniki, Greece), G. Theodorakopoulos and I.D. Petsalakis (Athens, Greece) 31

The nonplanarity of the ring and displacement of the substituent group in the orthogonal conformers of toluene, ethylbenzene, styrene and nitrosobenzene: a molecular orbital study
P. George, C.W. Bock, M. Trachtman (Philadelphia, PA, U.S.A.) and G.H. Penner (Winnipeg, Man., Canada) 37

MO theoretical calculations of EPR parameters of vanadium compounds. Part 1. CNDO/2 calculations of **g** tensors and anisotropic hyperfine structure tensors (**B**) of vanadium-containing compounds
F. Ritschl and H. Haberlandt (Berlin-Adlershof, G.D.R.) 45

Ab initio molecular orbital calculations of the IR spectra of hydrogen-bonded and lithium-bonded complexes of ammonia
J. Sadlej (Warsaw, Poland) 65

An ab initio study of the structural properties of β-substituted ethyl-free radicals
F. Bernardi (Bologna, Italy) and J. Fossey (Palaiseau, France) 79

Hartree–Fock instabilities in $(SN)_x$ systems: $(SN)_6$
M. Bénard (Strasbourg, France) and W.G. Laidlaw (Calgary, Alb., Canada) 95

Calculations of the conformational properties of acyclonucleosides. Part 2. Comparison of active and nonactive compounds
T.A. Wesolowski, A. Godzik and M. Geller (Warsaw, Poland) 105

On the electronic structure and conduction properties of aperiodic proteins: study of six-component polypeptide chains
A.K. Bakhshi, P. Otto and J. Ladik (Erlangen, F.R.G.) 113

Conformation, electrostatic potential and pharmacophoric pattern of GABA (gamma-aminobutyric acid) and several GABA inhibitors
D. Majumdar and S. Guha (Calcutta, India) 125

The vibrational spectrum of CH_2DNO_2
R. Engelke, D. Schiferl and W.L. Earl (Los Alamos, NM, U.S.A.) 141

Ab initio investigation of the nature of bonding in LiX dimers with first row substituents
A.B. Sannigrahi and T. Kar (Kharagpur, India) 149

Calculated structures and electrostatic potentials of some 1,4-dioxazines and 1,4-dioxadiazines
J.S. Murray and P. Politzer (New Orleans, LA, U.S.A.) 161

The geometry and internal rotational barrier of carbamic acid and several derivatives
M. Remko and S. Scheiner (Carbondale, IL, U.S.A.) 175

The bonding rules of Mo–Fe–S cluster compounds
C.-W. Liu, Z.-Y. Lin and J.-X. Lu (Fujian, People's Republic of China) 189

Theoretical analysis of the potential functions hindering the internal rotation of CHO–SH, CFO–SH and HO–NO
A. Toro-Labbé (Santiago, Chile) 209

Molesse d'un atome dans une molecule et definition de la mollesse d'un groupement fonctionnel: une echelle LCAO
M. Giambiagi, M.S. de Giambiagi, J.M. Pires et P. Pitanga (Rio de Janeiro, RJ, Brasil) 223

RHF and UHF MINDO/3 study on the molecular structures of galvinoxyl and *N*-galvinoxyl radicals
O. Kikuchi, O. Takahashi, K. Morihashi and M. Nakayama (Tsukuba, Japan) 233
Ab initio molecular orbital calculations of the infrared spectra of interacting water molecules. Part 1. Complexes of water with nitrogen, neon and argon
M.J. Bräsler, V.C.E. Carr, M.G. Gerazounis, N.R. Jugga, G.A. Yeo and T.A. Ford (Johannesburg, South Africa) 241
Medium effects on the molecular electronic structure. Part 2. The application of the theory of medium effects in the framework of the CNDO and INDO methods
H. Hoshi, M. Sakurai, Y. Inoue and R. Chûjô (Tokyo, Japan) 267
A quantum chemical study of the electroreduction of 2-cyclohexen-1-one
J.J. Nova and E. Brillas (Barcelona, Spain) 283
Structures and energies in some simple germylenes, GeXY (X,Y=H,F,Cl): a test of the MIDI-1 basis set
M.C. Kerins, N.J. Fitzpatrick (Dublin, Ireland) and M.T. Nguyen (Groningen, The Netherlands) 297
Increased valence theory and the four electron reduction of O_2 to H_2O
A. van der Putten, A. Elzing, W. Visscher, E. Barendrecht (Eindhoven, The Netherlands) and R.D. Harcourt (Parkville, Vic., Australia) 309
Molecular orbital calculations on anthrone
T. Schaefer and R. Sebastian (Winnipeg, Man., Canada) 319
Molecular orbital description of the polythiazyl polymer. Part 2. MNDO calculations of a structure with chlorine as a model dopant
L.A. Soares II, R.H. de A. Santos and M. Trsic (São Carlos, Brasil) 325
Benzenoid hydrocarbons with trigonal symmetry: enumeration and Kekulé structure counts
S.J. Cyvin, J. Brunvoll and B.N. Cyvin (Trondheim, Norway) 329
Ab initio studies of structural features not easily amenable to experiment. Part 62. The 4-21G optimized structure of the steroid, 4,4-dimethylandrostan-3-one
C. van Alsenoy (Wilrijk, Belgium), K. Wolinski, K. Siam and L. Schäfer (Fayetteville, AR, U.S.A.) 343
On the structure of the BH_4 radical and its potential energy surface for rearrangement and dissociation: an ab initio MO study
M.N. Paddon-Row and S.S. Wong (Kensington, N.S.W., Australia) 353

Short communications
Theoretical modelling of pyrolysis reactions: thermal; retroaldol reactions of β-hydroxy compounds
J. Kao (Richmond, VA, U.S.A.) 383
Quantumchemical (MNDO SCF/CI) calculations of the chiroptical properties of twisted conjugated diene and dione chromophores
Rejoinder to a comment
M.C.A. Donkersloot and H.M. Buck (Eindhoven, The Netherlands) 389

Book reviews 391

Author index 393

Subject index 394